

THEORY PROGRAM PUBLICATIONS – FY2014

Lead PI Steve Louie

Primary Publications

1. "Evolution of Interlayer Coupling in Twisted MoS₂ Bilayers", K. Liu, L. Zhang, T. Cao, C. Jin, D. Qiu, Q. Zhou, A. Zettl, P. Yang, S. G. Louie, and F. Wang, *Nature Commun.* vol. 5, p. 4966, **2014**. DOI: 10.1038/ncomms5966.
2. "Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor", M. M. Ugeda, A. J. Bradley, S.-F. Shi, F. H. da Jornada, Y. Zhang, D. Y. Qiu, W. Ruan, S.-K. Mo, Z. Hussain, Z.-X. Shen, F. Wang, S. G. Louie, M. F. Crommie, *Nature Materials* **2014**. DOI: 10.1038/nmat4061.
3. "Probing excitonic dark states in single-layer tungsten disulphide", Z. Ye, T. Cao, K. O'Brien, H. Zhu, X. Yin, Y. Wang, S. G. Louie, and X. Zhang, *Nature* vol. 513, p. 214-218, **2014**. DOI: 10.1038/nature13734.
4. "Control of single-molecule junction conductance of porphyrins via transition metal center", Z.-F. Liu, S. Wei, H. Yoon, O. Adak, I. Ponce, Y. Jiang, W.-D. Jang, L. M. Campos, L. Venkataraman, and J. B. Neaton, *Nano Lett.* vol. 14, p. 5365, **2014**. DOI: 10.1021/nl5025062.
5. "Charge transport and rectification in molecular junctions formed with carbon-based electrodes", T. Kim, Z.-F. Liu, C. Lee, J. B. Neaton, and L. Venkataraman, *Proc. Natl. Acad. Sci.*, vol. 111(30), **2014**. DOI: 10.1073/pnas.1406926111.
6. "Charge transport and rectification in molecular junctions formed with carbon-based electrodes", T. Kim, Z.-F. Liu, C. Lee, J. B. Neaton, and L. Venkataraman, *Proc. Natl. Acad. Sci.* vol. 111, p. 10928, **2014**. DOI: 10.1073/pnas.1406926111.
7. "Simultaneous Determination of Structures, Vibrations, and Frontier Orbital Energies from a Self-Consistent Range-Separated Hybrid Functional", I. Tamblyn, S. Refaelly-Abramson, J. B. Neaton, and L. Kronik, *J. Phys. Chem. Lett.* vol. 5, p. 2734, **2014**. DOI: 10.1021/jz5010939.
8. "Underdoped superconducting cuprates as topological superconductors", Y.M. Lu, T. Xiang and D.H. Lee, *Nature Physics* vol. 10, p. 634, **2014**. DOI: 10.1038/nphys3021.
9. "Electron Supercollimation in Graphene and Dirac Fermion Materis Using One-dimensional Disorder Potentials", S.K. Choi, C.-H. Park, and S.G. Louie, *Phys. Rev. Letters* vol. 113, p 026802, **2014**. DOI: 10.1103/PhysRevLett.113.026802.
10. "Tuning Many-body Interactions in Graphene: The Effects of Doping on Excitons and Quasiparticle Lifetimes", K. F. Mak, F. H. da Jornada, K. He, J. Deslippe, N. Petrone, J. Hone, J. Shan, S. G. Louie, and T. F. Heinz, *Phys. Rev. Lett.* vol. 112, p. 207401, **2014**. DOI: 10.1103/PhysRevLett.112.207401.
11. "Controlled formation of metastable germanium polymorphs", B. Haberl, M. Guthrie, B.D. Malone, J.S. Smith, S.V. Sinogeikin, M.L. Cohen, J.S. Williams, G.

- Shen, and J.E. Bradby, *Phys. Rev. B* vol. 89, p. 144111, **2014**. DOI: 10.1103/PhysRevB.89.144111.
12. "Band Offsets in c-Si/Si-XII Heterojunctions", J.I. Mustafa, B.D. Malone, [M.L. Cohen](#), and [S.G. Louie](#), *Solid State Comm.* vol. 191, p. 6, **2014**. DOI: 10.1016/j.ssc.2014.04.011.
13. "Gapped symmetric edges of symmetry protected topological phases", Y.M. Lu and [D.H. Lee](#), *Phys. Rev. B* vol. 89, p. 205117, **2014**. DOI: 10.1103/PhysRevB.89.205117.
14. "Systematic Determination of Absolute Absorption Cross-Section of Individual Carbon Nanotubes", K. Liu, X.P. Hong, S.K. Choi, C.H. Jin, R.B. Capaz, J. Kim, W. L. Wang, X.D. Bai, [S.G. Louie](#), E.G. Wang and [F. Wang](#), *Proc. of the Natl. Acad. of Sci.* vol. 111, p. 7564, **2014**. DOI: 10.1073/pnas.1318851111.
15. "Satellite Structures in the Spectral Functions of the Two-dimensional Electron Gas in Semiconductor Quantum Wells: A GW Plus Cumulant Study", J. Lischner, D. Vigil-Fowler, and [S.G. Louie](#), *Phys. Rev. B* vol. 89, p. 125430, **2014**. DOI: 10.1103/PhysRevB.89.125430.
16. "An efficient atomistic quantum mechanical simulation on InAs band-to-band tunneling field-effect transistors", Z. Wang, X.W. Jiang, S.S. Li, [L.W. Wang](#), *Appl. Phys. Lett.* vol. 104, p. 123504, **2014**. DOI: 10.1063/1.4869461.
17. "Doping dependence of the anisotropic quasiparticle interference in NaFe_{1-x}Co_xAs iron-based superconductors", P. Cai, W. Ruan, X. Zhou, C. Ye, A. Wang, X. Chen, [D.H. Lee](#) and Y. Wang, *Phys. Rev. Lett.* vol. 112, p. 127001, **2014**. DOI: 10.1103/PhysRevLett.112.127001.
18. "Hole transfer dynamics from a CdSe/CdS quantum rod to a tethered ferrocene derivative", K. Tarafder, Y. Surendranath, J.H. Olshansky, [A.P. Alivisatos](#), [L.W. Wang](#), *J. Am. Chem. Soc.* vol. 136, p. 5121, **2014**. DOI: 10.1021/ja500936n.
19. "Voltage tuning of vibrational mode energies in single-molecule junctions", Y. Li, P. Doak, L. Kronik, [J. B. Neaton](#), and D. Natelson, *Proc. Natl. Acad. Sci.* vol. 111, p. 1282, **2014**. DOI: 10.1073/pnas.1320210111.
20. "Determination of Energy Level Alignment and Coupling Strength in 4,4'-Bipyridine Single-Molecule Junctions", T. Kim, P. Darancet, J. R. Widawsky, M. Kotiuga, S. Y. Quek, [J. B. Neaton](#), and L. Venkataraman, *Nano Lett.* vol. 14, p. 794, **2014**. DOI: 10.1021/nl404143v.
- Acknowledgement: This work was supported primarily by the NSF MIRT program under award the DMR-1122594. Portions of this work were performed at the Molecular Foundry and supported by the Division of Materials Sciences and Engineering (Theory FWP), both under the auspices of the Office of Basic Energy Sciences of the U.S. Department of Energy under contract no. DE-AC02-05CH11231. We thank the National Energy Research Scientific Computing center for computational resources.
21. "Enhancement of band-to-band tunneling in mono-layer transition metal dichalcogenides two-dimensional materials by vacancy defects", X.W. Jiang, J. Gong, N. Xu, S.S. Li, [L.W. Wang](#), *Appl. Phys. Lett.* vol. 104, p. 023512, **2014**. DOI:

10.1063/1.4862667.

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22. "Insight into the photoelectron angular dependent energy distribution of negative-electron-affinity InP photocathodes", Z. Chen, X. Jiang, S. Dong, J. Li, S.S. Li, [L.W. Wang](#), *App. Phys. Lett.* vol. 104, p. 021120, **2014**. DOI: 10.1063/1.4862645.
23. "Importance of Oxygen Octahedra Tilts for the Electron-phonon Coupling in K-doped BaBiO₃", T. Bazhirov, S. Coh, [S.G. Louie](#), and [M.L. Cohen](#), *Phys. Rev. B* vol. 88, p. 224509, **2013**. DOI: 10.1103/PhysRevB.88.224509.
24. "Tuning Rectification in Single-Molecular Diodes", A. Batra, P. T. Darancet, Q. Chen, J. Meisner, J. R. Widawsky, [J. B. Neaton](#), C. Nuckolls, and L. Venkataraman, *Nano Lett.* vol. 13, p. 6233, **2013**. DOI: 10.1021/nl403698m.

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25. "Optical Spectrum of MoS₂: Many-body Effects and Diversity of Exciton States", D.Y. Qiu, F.H. da Jornada, and [S.G. Louie](#), *Phys. Rev. Lett.* vol. 111, p. 216805, **2013**. DOI: 10.1103/PhysRevLett.111.216805.
26. "Plane-Wave based electron tunneling through field emission resonance states", A Garcia-Lekue, D. Sanchez-Portal, A. Arnaud, [L.W. Wang](#), *Phys. Rev. B* vol. 88, p. 155441, **2013**. DOI: 10.1103/PhysRevB.88.155441.

Secondary Publications

1. "Ytterbium-driven strong enhancement of electron-phonon coupling in

- graphene", C. Hwang, D. Y. Kim, D. A. Siegel, K. T. Chan, J. Noffsinger, A. V. Fedorov, M. L. Cohen, B. Johansson, J. B. Neaton, and A. Lanzara, *Phys. Rev. B* vol. 90, p. 115417, **2014**. DOI: 10.1103/PhysRevB.90.115417.
2. "Carbon kagome lattice and orbital-frustration-induced metal-insulator transition for optoelectronic", Y. Chen, Y.Y. Sun, H. Wang, D. West, Y. Xie, J. Zhong, V. Meunier, M. L. Cohen, and S. B. Zhang, *Phys. Rev. Lett.* vol. 113, p. 085501, **2014**. DOI: 10.1103/PhysRevLett.113.085501.
 3. "Ab Initio Study of Hot Carriers in the First Picosecond after Sunlight Absorption in Silicon", M. Bernardi, D. Vigil-Fowler, J.B. Neaton, and S.G. Louie, *Phys. Rev. Lett.* vol. 112, p. 257402, **2014**. DOI: 10.1103/PhysRevLett.112.257402.
 4. "Revealing the atomic restructuring of Pt-Co nanoparticles", H. Xin, S. Alayoglu, R. Tao, A. Genc, C.M. Wang, L. Kovarik, E.A. Stach, L.W. Wang, M. Salmeron, G. Somorjai, H. Zheng, *Nano Lett.* vol. 14, p. 3203 (2014).
 5. "Lattice matching and electronic structure of finite-layer graphene/h-BN thin films", Y. Sakai, S. Saito, and M.L. Cohen, *Phys. Rev. B* vol. 89, p. 115424, **2014**. DOI: 10.1103/PhysRevB.89.115424.
 6. "First-principles DFT+GW Study of Oxygen Vacancies in Rutile TiO₂", A. Malashevich, M. Jain, and S.G. Louie, *Phys. Rev. B* vol. 89, p. 075205, **2014**. DOI: 10.1103/PhysRevB.89.075205.
 1. "Effect of Spin Fluctuations on Quasiparticle Excitations: First-principles Theory and Application to Sodium and Lithium", J. Lischner, T. Bazhirov, A.H. MacDonald, M.L. Cohen, and S.G. Louie, *Phys. Rev. B* vol. 89, p. 081108, **2014**. DOI: 10.1103/PhysRevB.89.081108.
 2. "Tunable Charge Transport in Single-Molecule Junctions via Electrolytic Gating", B. Capozzi, Q. Chen, P. Darancet, M. Kotiuga, M. Buzzo, J. B. Neaton, C. Nuckolls, and L. Venkataraman, *Nano Lett.* vol. 14, p. 1400, **2014**. DOI: 10.1021/nl404459q.
 3. "Electron-phonon coupling and superconductivity in Li-intercalated layered borocarbide compounds", T. Bazhirov, Y. Sakai, S. Saito, and M.L. Cohen, *Phys. Rev. B* vol. 89, p. 045136, **2014**. DOI: 10.1103/PhysRevB.89.045136.
- Acknowledgement: This work was supported by the National Science Foundation Grant No. DMR10-1006184 and by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the Lawrence Berkeley National Laboratory and the Department of Energy's NERSC supercomputing facility. Numerical calculations were also partly carried out on the TSUBAME2.0 supercomputer at the Tokyo Institute of Technology. Y.S. acknowledges financial support from Japan Society for the Promotion of Science (12J08928). T.B. acknowledges support from NSF award COINS EEC-0832819.
7. "Ab Initio Quasiparticle Band Structure of ABA- and ABC-stacked Graphene Trilayers", M.G. Menezes, R.B. Capaz, and S.G. Louie, *Phys. Rev. B* vol. 89, p. 035431, **2014**. DOI: 10.1103/PhysRevB.89.035431.

4. "Local Electronic and Chemical Structure of Oligo-acetylene Derivatives Formed Through Radical Cyclizations at a Surface", A. Riss, S. Wickenburg, P. Gorman, L.Z. Tan, H.-Z. Tsai, D.G. de Oteyza, Y.-C. Chen, A.J. Bradley, M.M. Ugeda, G. Etkin, [S.G. Louie](#), F.R. Fischer, and [M.F. Crommie](#), *Nano Lett.* vol. 14, p. 2251, **2014**. DOI: 10.1021/nl403791q.
5. "Using light-switching molecules to modulate charge mobility in a quantum dot array", I.H. Chen, J. Trinastic, [L.W. Wang](#), H.P. Cheng, *Phys. Rev. B* vol. 89, p. 115415, **2014**. DOI: 10.1103/PhysRevB.89.115415.
6. "Altered magnetism and new electronic length scales in magneto-electric La₂/3Sr₁/3MnO₃-BiFeO₃ heterointerface", S.K. Mishra, D. Mazumdar, K. Tarafdar, [L.W. Wang](#), S.D. Kevan, C. Sanchez-Hanke, A. Gupta, [S. Roy](#), *New Journal of Phys.* vol. 15, p. 113042, **2013**. DOI: 10.1088/1367-2630/15/11/113042.
7. "Theory of the Raman Spectrum of Rotated Double-layer Graphene", S. Coh, L.Z. Tan, [S.G. Louie](#), and [M.L. Cohen](#), *Phys. Rev. B* vol. 88, p. 165431, **2013**. DOI: 10.1103/PhysRevB.88.165431.
8. "Hexagonal germanium formed via a pressure-induced phase transformation of amorphous germanium under controlled nanoindentation", J.S. Williams, B. Haberi, S. Keshmukh, B.C. Johnson, B.D. Malone, [M.L. Cohen](#), and J.E. Bradby, *Phys. Status Solidi (RRL)* vol. 7, p. 355, **2013**. DOI: 10.1103/PhysRevB.88.165431.